Next Level Python

Tips, tool, and techniques for being highly productive in Python

Topics

Prelude
Data structures
Iterators
Functions, Files, & Modules
Exercises

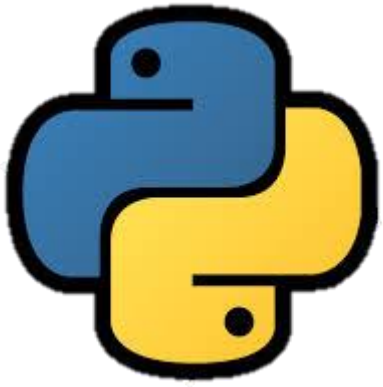
Using an IDE
Debugging
Conda Environments
Exercises

Code snippets, if you want to follow along:

bit.ly/2ScFewN

Topic 0

Prelude



Prelude

What is Python?

- Invented in the early ‘90s by Guido Van Rossum

~~BDFL~~

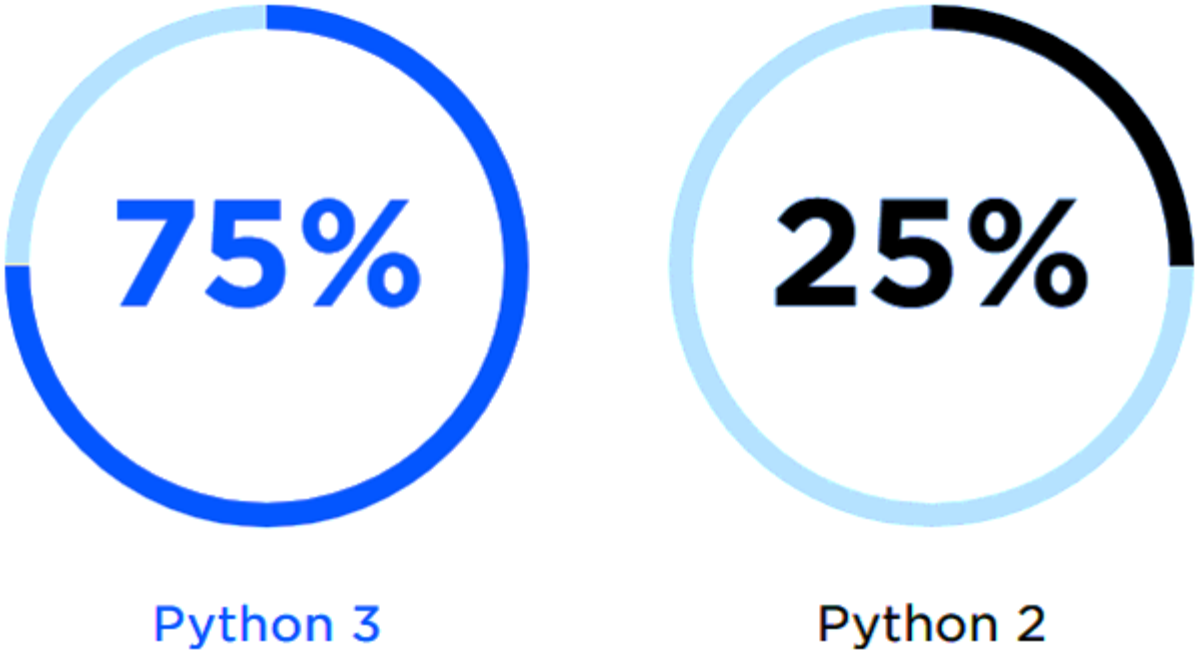
- **CPython Interpreter**
  - Reads your code 📖
  - Parses it 👀
  - Checks for **syntax** errors ✔
  - Generates **instructions** 👉
  - Steps through instructions ⏭

Prelude

2 vs. 3

Python 3 > Python 2

Stick to 3.5+

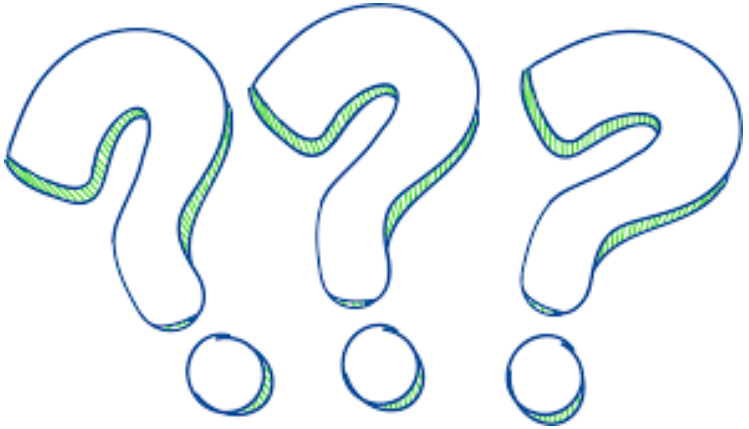


source: opensource.com

Prelude
Variables

- Sounds simple, but worth clarifying

```
3       a = 1
4       a = 2
```



What just happened?

Did we change 1? Or a?

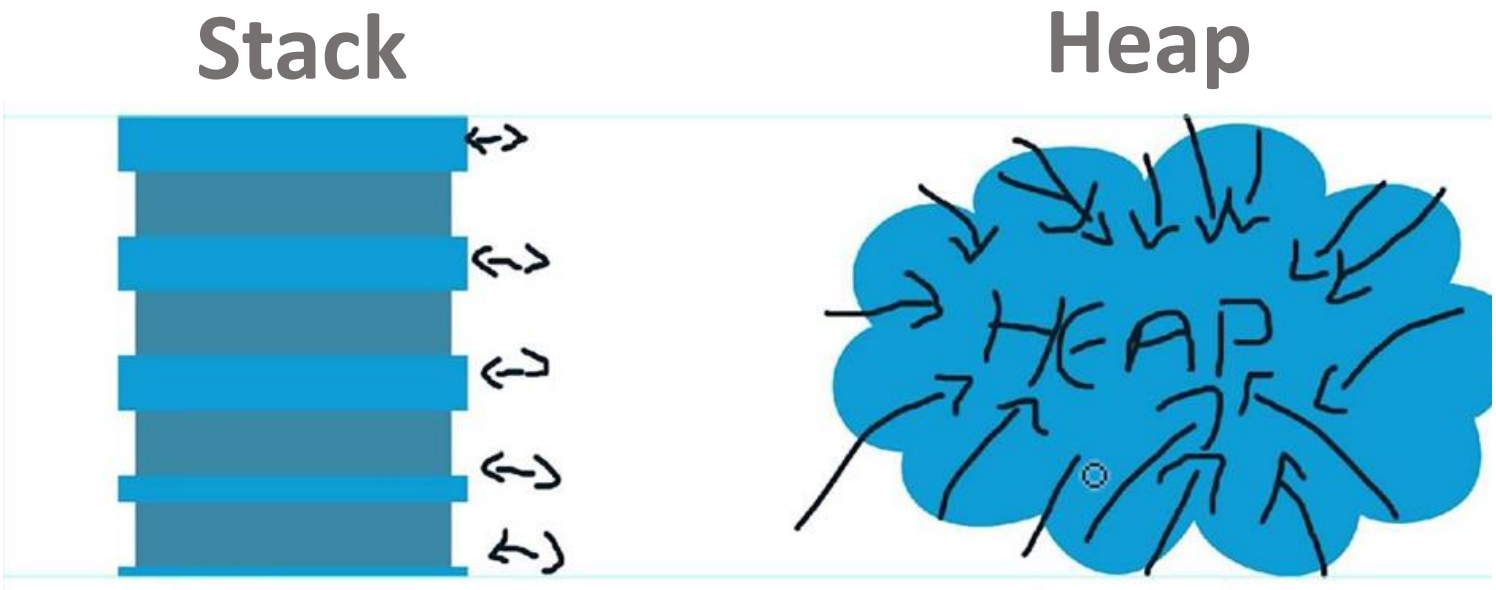
What happened to 1?

Prelude

Variables

```
3      a = 1
4      a = 2
```

- Values are **objects**
  - **objects** live on the heap
- Names tell you how to find an object
  - **names** live on the heap



Prelude

Variables

```
3    foo = [3,1,2]
4    bar = sort(foo)
5    print(foo)
6    # [1,2,3]
```

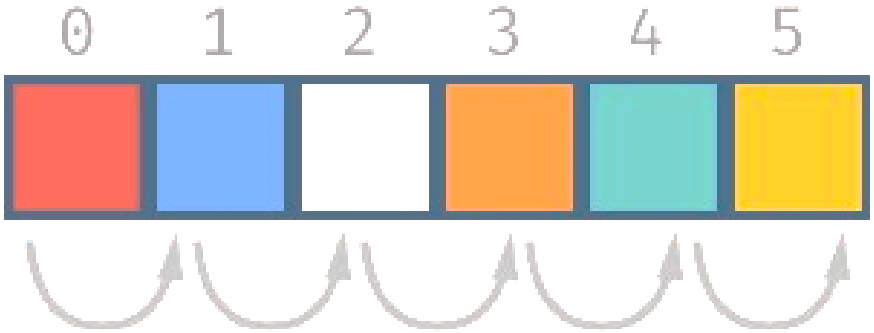
What happened to foo?

Prelude

Beyond CPython

- There are other ways of running your Python code:

The best way to get CPython + Scientific libraries



Topic 1

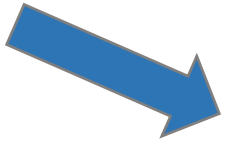
Data Structures

Topic 1

Data Structures

Lists

- Most of us are familiar
- Store data in **order**
- Can **loop** through
- Can look up by **index**



```
abc = [1,2,3]
print(abc[2])  # 3
```

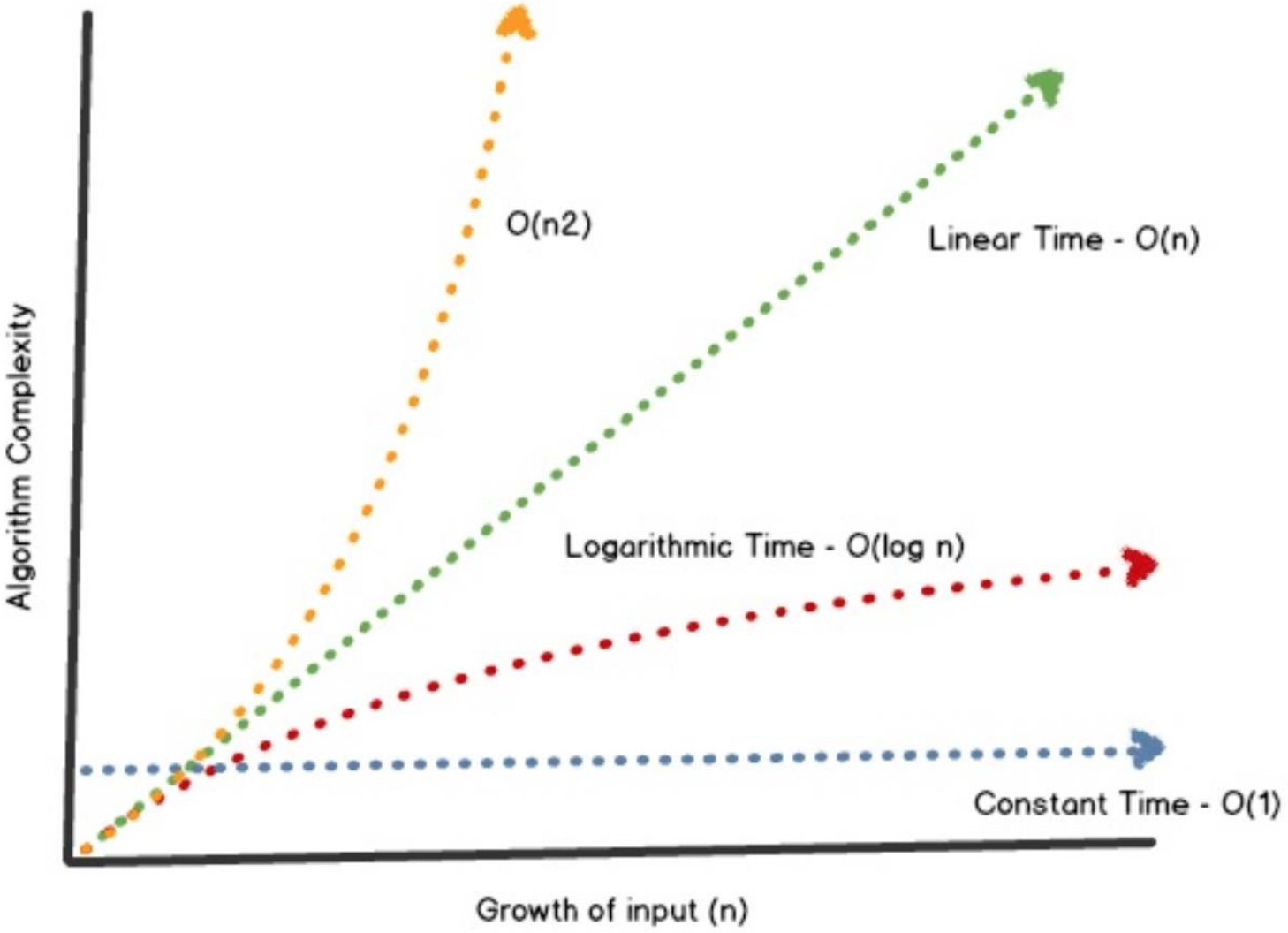
- Slow **searching**

Data Structures

Dictionaries

- Store data as key: value pairs
  - Keys can be:
    - Numbers
    - Strings
    - Tuples of numbers, strings
  - Values can be: anything!
  - "**Instant**" lookup by key!
    - O(1) even if 1e6 entries!
  - Slower than lists for looping

Data Structures
Dictionaries



Data Structures

Dictionaries

- Use cases:
  - Store properties of something in one place
- Example:

```
my_particle = {
    'x': 12.0,
    'y': 13.5,
    'z': -12.0,
}

def print_particle(particle_dict):
    print("x: ", particle_dict['x'])
    print("y: ", particle_dict['y'])
    print("z: ", particle_dict['z'])
```

Data Structures
Dictionaries

- Use cases:
  - Data you have to access by a name or ID
  - Catalogs
  - Filenames for datasets
- Example:

```
30  runs_data_number = {
31      'M29-768': 345
32      'M35-1536': 138
33      ...
34  }
35
36  print(runs_data_number['M35-1536'])  # 138
37
38  for run in dataset:
39      run_number = runs_data_number[run]
40      file = open(run + '/' + data_number, 'r')
41      ...
```

Data Structures

Dictionaries – Trick!

- You can use tuples as dictionary keys
- Use this as a sparse matrix, esp. for non-numerical data!

```
17  # Dictionaries as matrix/table
18  mat = {}
19  mat[(1, 9)] = 5
20  mat[(23000, 1e12)] = 4
21  for (keya, keyb) in mat.keys():
22      val = mat[(keya, keyb)]
23      print(f"a: {keya}  b: {keyb}  val: {val}")
24  # Output:
25  # a: 1  b: 9  val: 5
26  # a: 23000  b: 1000000000000.0  val: 4
```

- This would require on the order of 2TB of RAM if you used a list!
- Great way to store values that belong at the intersection of two other things, e.g. (computer A, and computer B) have an open connection C

Data Structures

Dictionaries – Trick!

- You can use dictionaries to hold arguments for functions, apply them later

```
111  # Dictionaries: Tip for Function arguments
112  def myfunc(min, max, step):
113      pass
114
115  kwargs = {"min": 0, "max": 10, "step": 14}
116  myfunc(**kwargs)
117
118  all_the_args = [
119      {"min": 0, "max": 10, "step": 3},
120      {"min": 0, "max": 12, "step": 4},
121      {"min": 6, "max": 10, "step": 1}
122  ]
123  for kwargs in all_the_args:
124      myfunc(**kwargs)
```

Data Structures
Dictionaries – Tip!

- You can use lists, and other dictionaries *inside* dictionary values!

```
28  # Dictionaries with lists for values
29  # Table of companions for some galaxy
30  galaxies = ["M31", "MW"]
31
32  companions = {}
33  companions["M31"] = ["M32", "M110", "etc"]
34  companions["MW"] = ["CMd", "LMC", "SMC", "etc"]
35
36  for galaxy in galaxies:
37      cs = companions[galaxy]
38      print(f"{galaxy} has {len(cs)} companions!")
39  # M31 has 3 companions!
40  # MW has 4 companions!
```

Data Structures

Dictionaries – Technique!

- If you're calling some function, e.g. from matplotlib lots of times with slight differences, use a dictionary to hold defaults

```
130   my_defaults = {
131       "marker": "o",
132       "color": "blue",
133       "linewidth": 3,
134       "alpha": 0.6
135   }
136
137   plot([1, 2, 3], **my_defaults)
138   plot([3, 4, 5], **my_defaults)
```

Better yet! Make a function!

Data Structures

Sets

- Sets are like a "**bag**" of values
- Values can be strings, numbers, tuples, etc.
- Values are unique.
  - Adding the same thing twice has no effect
- Not ordered

- **"instant"** adding and removing values
- **"instant"** membership testing
- Operations for
  - Testing
  - Grouping
  - Differencing
  - etc.

Data Structures

Sets

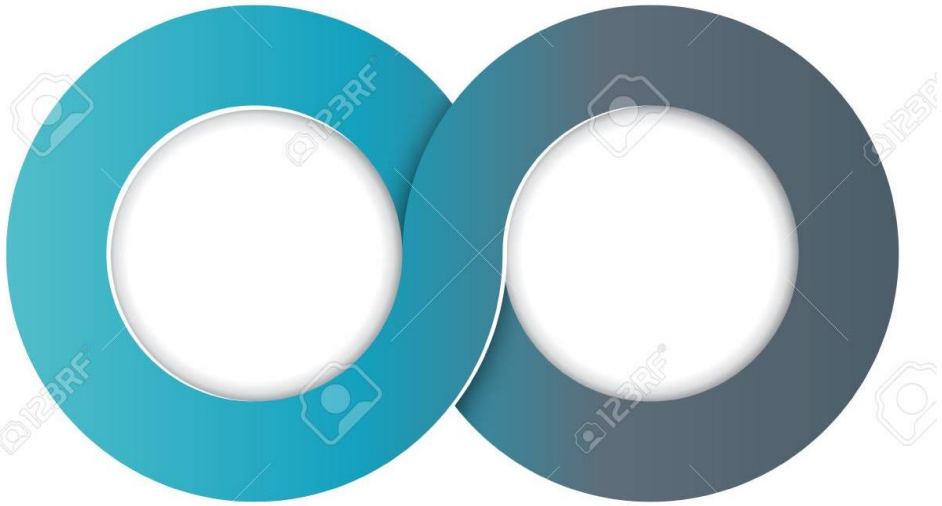
- Use case:
  - You have a data set, with some possibly overlapping groups
  - You want to focus on one group at a time
  - Solution: Put the group in a set
  - You can easily isolate just the data in the group

Data Structures
Sets

```
15  bar = set()  # or {,}
16  bar.add(1)
17  bar.add(2)
18
19  print(2 in bar)  # True
20  print(3 in bar)  # False
21
22  baz = set([2,3,4])
23  print(bar & baz)  # {2}       in both
24  print(bar | baz)  # {1,2,3,4} in either
25  print(bar ^ baz)  # {1,3,4}   in either, but not both!
26  print(bar > baz)  # False     is everythin in bar, also in baz?
```

Topic 2

Iterators



Topic 2

Iterators

- Generators create “lazy sequences”, called iterators

```
60    foo = range(0, 1000000000000, 1)
61    for b in foo:
62        print(b)
63        if b > 10:
64            break
```

This **works**!

Why doesn’t my computer crash?

Iterators

Behind the scenes

- Behind the scenes, they are a function that returns more than one value.
  - Every time you run the function, you get the next value!

Definition:

```
66  def count_down(stop):
67      value = 0
68      while value > stop:
69          yield value
70          value -= 1
```

Usage:

```
72  for i in count_down(-5):
73      print(i, end=', ')
74  print()
75  # 0, -1, -2, -3, -4
```

Iterators
Useful Iterator Functions

- enumerate
  - Loop through things with indexes

```
78    # Iterators: enumerate
79    letters = ['a', 'b', 'c', 'd', 'e']
80
```

Iterators
Useful Iterator Functions

- zip
  - Group items from multiple lists into tuples

```
letters = ['a', 'b', 'c']
numbers = [5, 4, 3]

list(zip(letters, numbers))
# [('a', 5), ('b', 4), ('c', 3)]

for letter, number in zip(letters, numbers):
    print(letter + str(number))
# a5
# b4
# c3
```

Iterators
Useful Iterator Functions

- zip
  - Trick! You can *un*zip as well, using *

```
107    # Zip trick
108    print(zipped)       # [('a', 5), ('b', 4), ('c', 3)]
109    print(list(
110        zip(*zipped)    # (['a', 'b', 'c'], [1,2,3])
111    ))
```

Iterators
Useful Iterator Functions

- map, filter, etc
  - Really useful for lists, but if using numpy there are better better ways

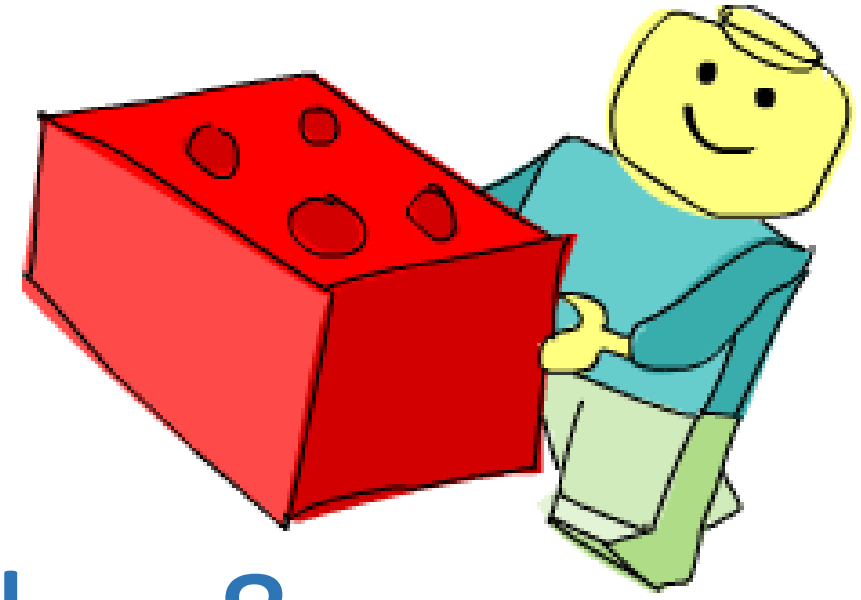
Iterators
Generator Expressions

- Generator comprehensions by example

```
 8    # Make a sequence from 0 to 10^18
 9    gen1 = range(1, 1000000000000000000)
10    # Square them all
11    gen2 = (i ** 2 for i in gen1)
12    # Include only odd numbers
13    gen3 = (i for i in gen2 if i % 2 == 0)
14    # Enumerate them all
15    gen4 = enumerate(gen3)
16
17    for i, value in gen4:
18        print(i, value)
19        if value > 120:
20            break
```

Prints:

```
0 4
1 16
2 36
3 64
4 100
5 144
```



Topic 3

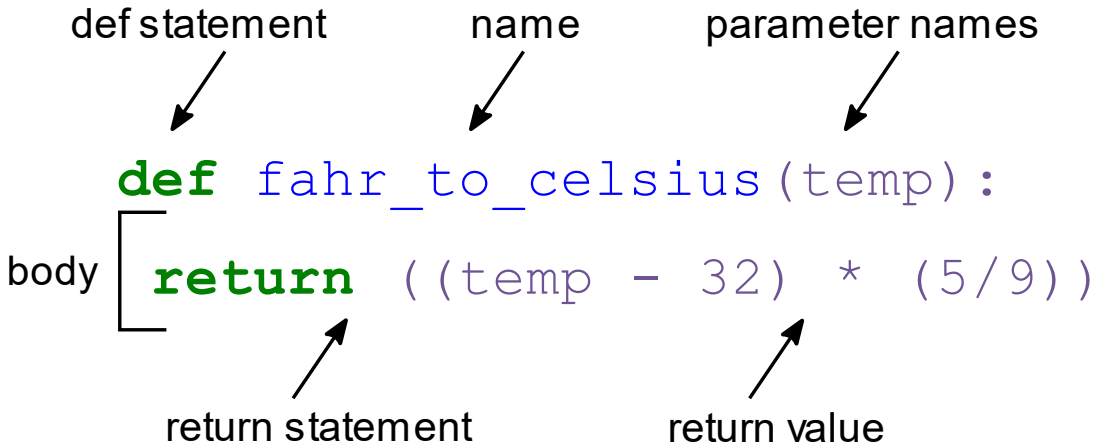
Functions, Files & Modules

Oh, and packages too

Topic 3

Functions

- **DRY**: Do not Repeat Yourself
  - Use functions to pull out repeated code, patterns
- **Safety**
  - Variables inside functions can't **leak** out
  - Easier variable naming
- **Abstraction**
  - Once you've written one type of data analysis, don't need to worry about the details again



Functions

Rules of Thumb

Create a function if:

- You write the same thing 2 or more times
- You know it will change in the future
- It was tricky to get right

```
theta = arctan2(sqrt(x**2 + y**2),z) * 180/np.pi
phi = arctan2(y,x) * 180/np.pi + 180
```

- It's a step in a data analysis pipeline

```
data1    = read_in_data(...)
data2    = read_in_data(...)
merged   = match_data(data1, data2)
reduced  = analyze_data(merged)
plot_data(reduced)
```

Rules of Thumb

- Split up a function if:
  - It has more than ~10 lines (industry)
  - It has more than about **two loops** (science)
  - It takes more than ~5 parameters
  - It does two different things, based on a parameter
- Prefer two, or three simple functions over one big one

Functions

Rules of Thumb

- “Magic Functions”
  - It does different things, based on parameters

- Symptoms:
  - 19+ parameters
  - Some parameters can’t be used with others
  - matplotlib...

IMO scientists are particularly prone to this

Split it up!

Functions

Decorators

```
@np.vectorize
```

- Put this above your function, and it will work on arrays

- Lots of other use cases for decorators, but this is the one I use on a daily basis

Functions
Docstrings

- Explain what your function does!

```
[3]: mf.get_rprof_set_run()
```

```
Signature: mf.get_rprof_set_run(run)
Docstring:
Get the radially averaged data sets for some run name.

>>> get_rprof_run('M29-768')
File:      /user/scratch14.4/wthompson/PyPPM/momsfunctions.py
Type:      function
```

```
[ ]:
```

Functions: Docstrings

```
def galactocentric_distance(heliocentric_dist, galactic_long, galactic_lat):
    """\
    Calculate the galactocentric distance of an object

    ## INPUT
    * Heliocentric distance
    * galactocentric longitude
    * galactrocentric latitude

    ## OUTPUT
    * Galactocentric distance (same as input units)

    Citation: Tobias Westmeier, 2018
    http://www.atnf.csiro.au/people/Tobias.Westmeier/tools_coords.php

    ## EXAMPLES
    >>> galactocentric_distance(50.0, -57.2, -44.1)
    43.495214885473814

    >>> galactocentric_distance(13.0, -5.2, +19.1)
    11.464307213925464
    """

    component_1 = heliocentric_dist * math.cos(galactic_lat) * math.cos(galactic_long) - sun_galaxy_d
    component_2 = heliocentric_dist * math.cos(galactic_lat) * math.sin(galactic_long)
    component_3 = heliocentric_dist * math.sin(galactic_lat)

    galact_dist = (component_1 ** 2 + component_2 ** 2 + component_3)**0.5
```

Functions
Doc-tests?

- Explain what your function does!

```
[3]: mf.get_rprof_set_run()

[ ]:
```

```
Signature: mf.get_rprof_set_run(run)
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Type:      function
```

Topic 3

Files & Modules

- Make a text file, give it a **.py** extension
- Congrats, you made a module!

Topic 3

Files & Modules

- Make a text file, give it a **.py** extension
- Congrats, you made a module!

- Any python file is a **module** that can be **import**ed
- Python looks for modules in your current directory, and PYTHONPATH (that's where e.g. numpy is)

- If you want to find where a module is:
  - Import it, and `print(somemodule).__file__`

Topic 3

Files & Modules

- Importing things should have no side-effects
- At the top level, modules should only include:
  - Constants
  - Functions
  - Classes
- Bad design: importing the module makes a plot show up

Topic 3

Packages

- Put a group of modules in a folder
- Add a file named “__init__.py”
- Congrats, you have a package!

- Now you can group your modules together, e.g. scipy
- You could even publish your package to pypi

Exercises

- Make a function that:
  - Takes three arguments (x,y,z)
  - Returns the distance of the vector
- Make a function that:
  - Takes two points as dictionaries
  - Returns the distance between them
- Put your functions in a module
- Document them!
- Import your module, and use it!
- Extra: Make a function that works over numpy arrays of the vectors (@np.vectorize)

Topic 4

Using an IDE

IDEs

What can an IDE do for you?

- Syntax highlighting
- Multiple cursors
- Integrated terminal
- Warnings as you type (and in panel)
- Autocomplete
- Autoformat
- Code outlines
- Live code sharing, like Google Docs
- Debugging (more on this later)
- Version control (another session?)

Topic 5

Debugging

Debugging

Reading Stack Traces

- http://cs.franklin.edu/~ansaria/traceback.html

- Types of Exceptions
  - IndentationError
  - SyntaxError
  - IndexError
  - ValueError
  - TypeError
  - KeyboardInterrupt

- buggy-dictionaries.py

Debugging

Using a Debugger

- Breakpoints
- Stepping through
- Stepping in & stepping out
- Conditional breakpoints
- Logpoints
- Hitcounts

Topic 6

Conda Environments

Environments

- Reproducible science is important
- Your code should work the same way
  - Next year
  - On someone else's computer

- Installing a new version of a library shouldn't break your other code

Environments

- Most popular environment system is **virtualenv**
- For our use cases, **conda** is a good choice
  - Comes built in with Anaconda

- Use conda to create a new environment for each project with:
  - Different packages
  - Different versions of python

Conda Environments

- Create environment.yml
  - conda env create -f environment.yml
- List environments:
  - conda env list
- Activate an environment:
  - conda activate <env name>

Exercises

- Install an IDE
- Put in your functions from before
- Add a sneaky bug (not a syntax error)
- “Switch seats”, and try out the debugger on each others’ code